Coulomb Explosion Mechanisms for Ion Damage

Cynthia J. Olson Reichhardt, T-12

It has been known for many years that ion irradiation produces etchable damage tracks, which can be microns in length, in only some materials. The fact that most track-forming materials are insulators, while most metals do not form damage tracks, suggests that electronic processes play an important role in the ion-target interaction. This picture is too simple, however, since not all insulators form tracks equally well. The basic physics of the system was never fully unraveled even as demand for track-forming materials spurred a rapid empirical identification of materials that respond strongly to ion damage.

Numerous models have been developed over the years to explain track formation and sputtering processes, but each has suffered from limitations. One simple picture is to consider a collision cascade initiated when the impinging ion directly strikes a target atom, resulting in a series of collisions that progress through the lattice. Such direct atomic collisions would be expected to occur equally in metals and insulators. Thermal spike models, in which the energy deposited by the impinging ion is converted to lattice phonons that then locally melt the lattice over longer time scales, are also problematic since no correlations have been found between track formation and the thermal properties of the material.

The Coulomb explosion or ion explosion model has proven less popular than other models in spite of the fact that it could potentially reproduce the difference in damage between metals and insulators. In this model, the energy of the ion beam is assumed to lie in the electronic stopping regime. Here, the ion carries an effective charge because it loses those electrons with orbital velocity smaller than the velocity of the ion in the medium. As it passes through the target, the projectile ionizes atoms along its trajectory. These target ions then recoil under their mutual Coulomb repulsion. For example, the potential energy of two electron charges spaced at one interatomic distance is 3.5 eV, and a cluster of five ions has a Coulomb energy of about 30 eV. These amounts of repulsive energy are substantial compared to the binding energy per atom of the solid.

A Coulomb explosion process could be highly effective in destroying local lattice order along the track. The main barrier to the motion of target atoms out of their lattice registry positions is the presence of neighboring target atoms that are simply in the way. Target atoms undergo a decrease in their effective Pauling radius while ionized, due to the loss of electrons in their outer shells. This provides a significant amount of free volume in which the ionized target atoms can move, and permits much more extensive disordering of the lattice than is possible in typical vacancy production models. Furthermore, once the ionized target atoms deionize, they may be permanently trapped out of lattice registry, since thermal excitation is not sufficient to restore order to the lattice, in contrast to the possible recombination of interstitial and vacancy atoms that can occur in damage processes in the nuclear stopping regime.

A major concern with the Coulomb explosion model is the fact that the charge induced along the trajectory must persist long enough to allow significant motion of the target atoms to occur. It has normally been assumed that the time scale for target ion motion to occur is on the order of the inverse phonon frequency, 10^{-12} s. Even in insulating materials, it is likely that electrons from the material outside the strongly charged track region will be able to neutralize the charge in a time shorter than this. I have performed a theoretical estimation

of the radius and charge of the ionized track that would be produced by an ion in the electronic stopping regime. It is important to note that the track develops an intense charge due to the large amount of energy that is deposited on a very local scale by the impinging ion. Figure 1 shows an illustration of local energy deposition by a moving charge in a simulated charged system. Due to the strongly localized charge, a relatively narrow region of charged ions inside the track experience an intense accelerating force from the resulting electric field. This is sufficient to induce significant motion of the target ions on time scales of 10^{-15} s or shorter, long before thermal motion due to phonons can occur. It may be possible for the charge of the track to persist for times of this order, especially in insulating materials. This suggests that Coulomb explosion processes may be more effective than previously believed at producing damage tracks, and underscores the importance of considering direct Coulomb interactions between the target ions and the charged track region, rather than waiting for the energy deposited into the electronic degrees of freedom to thermalize.

For more information contact Cynthia J. Olson Reichhardt at cjrx@lanl.gov.
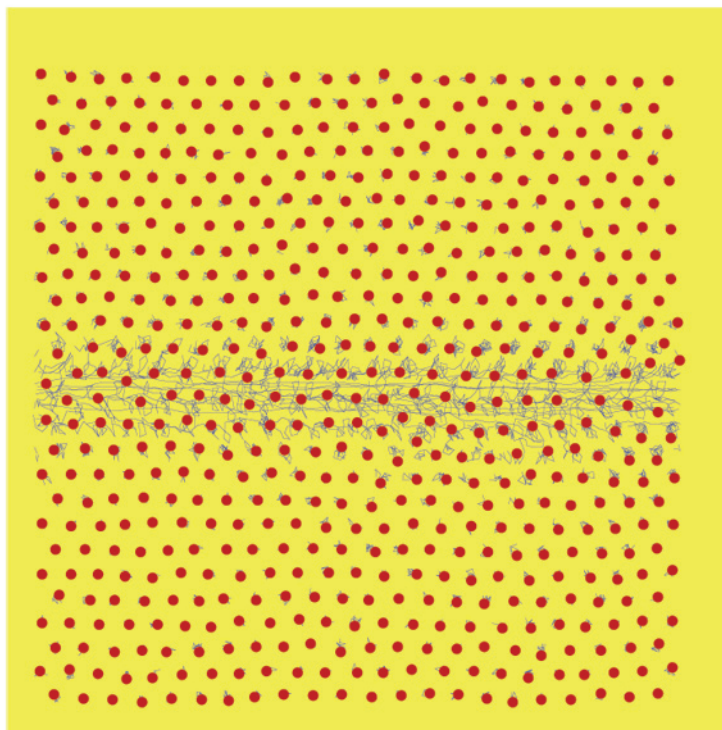
*Fig. 1.
Highly localized deposition of energy by moving charge in a strongly Coulomb interacting system of charges.*

Los Alamos
NATIONAL LABORATORY
— EST.1943 —